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Poisson's Ratio for Tetragonal Crystals

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ARL-TR-423

March 1995

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REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY *(Leave blank)*

2. REPORT DATE
March 1995

3. REPORT TYPE AND DATES COVERED
Technical Report

4. TITLE AND SUBTITLE
POISSON'S RATIO FOR TETRAGONAL CRYSTALS

5. FUNDING NUMBERS

6. AUTHOR(S)
Arthur Ballato

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
US Army Research Laboratory (ARL)
Electronics and Power Sources Directorate (EPSD)
ATTN: AMSRL-EP
Fort Monmouth, NJ 07703-5601

8. PERFORMING ORGANIZATION REPORT NUMBER
ARL-TR-423

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution is unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*
General expressions for Poisson's ratio are derived for tetragonal crystals; simplified forms are given for cases involving symmetry directions.

14. SUBJECT TERMS
Isotropic media; tetragonal symmetry

15. NUMBER OF PAGES
13

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT
Unclassified

18. SECURITY CLASSIFICATION OF THIS PAGE
Unclassified

19. SECURITY CLASSIFICATION OF ABSTRACT
Unclassified

20. LIMITATION OF ABSTRACT
UL

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POISSON'S RATIO FOR TETRAGONAL CRYSTALS

Abstract

General expressions for Poisson's ratio are derived for tetragonal crystals; simplified forms are given for cases involving symmetry directions.

Introduction

Poisson's ratio, ν, is defined for isotropic media as the quotient of lateral contraction to longitudinal extension arising from application of a simple tensile stress; in most materials, this dimensionless number is positive. In crystals, ν takes on different values, depending on the directions of stress and strain chosen. The ratio finds application in a variety of areas of applied elasticity and solid mechanics, for example, as indication of the mechanical coupling between various vibrational modes of motion.

The maximum value of $\nu = +1/2$ is obtained in the incompressible medium limit, where volume is preserved; for ordinary materials, values of $+1/4$ to $+1/3$ are typical, but in crystals ν may vanish, or take on negative values. Analytical formulas for Poisson's ratio are expressed in terms of elastic constants. For the case of crystals of general anisotropy, these expressions are quite unwieldy, but for tetragonal crystals the symmetry elements reduce the complexity considerably.

Crystals of tetragonal symmetry include a number of ferroelectrics as well as lithium tetraborate, a nonferroelectric with substantial piezoelectric coupling and temperature-compensated properties. These materials are potentially important for high technology applications such as cellular radio and microwave collision avoidance radar. Each of the seven tetragonal point groups is characterized by one of two elastic matrix schemes, so it is necessary to distinguish among the point groups. The distinction relates to symmetry: those groups that appear as holohedral under classical x-ray analysis (classes 4-bar 2m, 422, 4mm, and 4/m mm) have an elastic matrix in which c_{16} and s_{16} constants do not appear; the remainder (classes 4-bar, 4, and 4/m) retain the c_{16} and s_{16} entries. The presence of piezoelectricity is neglected.

Expressions Relating Tetragonal Stiffnesses and Compliances

Relations for Poisson's ratio are most simply expressed in terms of the elastic compliances $[s_{\lambda\mu}]$. It is often the case, however, that the most accurate determinations of the elastic constants (resonator and transit-time methods) yield values for the stiffnesses $[c_{\lambda\mu}]$ directly; the conversion relations are given below. For the tetragonal system, the elastic stiffness and compliance matrices have identical form. Referred to the x_k axes as defined in the IEEE Standard, the matrices are, including the c_{16} and s_{16} entries:

$$\begin{matrix} c_{11} & c_{12} & c_{13} & 0 & 0 & c_{16} \\ c_{12} & c_{11} & c_{13} & 0 & 0 & -c_{16} \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ c_{16} & -c_{16} & 0 & 0 & 0 & c_{66} \end{matrix} \qquad \begin{matrix} s_{11} & s_{12} & s_{13} & 0 & 0 & s_{16} \\ s_{12} & s_{11} & s_{13} & 0 & 0 & -s_{16} \\ s_{13} & s_{13} & s_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & s_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & s_{44} & 0 \\ s_{16} & -s_{16} & 0 & 0 & 0 & s_{66} \end{matrix}$$

Stiffness and compliance are matrix reciprocals; the seven independent components of each are related by:

$$s_{11} = [(c_{33} / C_1) + (c_{66} / C_2)] / 2 \; ; \; s_{12} = [(c_{33} / C_1) - (c_{66} / C_2)] / 2$$

$$(s_{11} + s_{12}) = [c_{33} / C_1] \; ; \; (s_{11} - s_{12}) = [c_{66} / C_2]$$

$$s_{13} = - [c_{13} / C_1] \; ; \; s_{16} = - [c_{16} / C_1]$$

$$s_{33} = [(c_{11} + c_{12}) / C_1] \; ; \; s_{66} = [(c_{11} - c_{12}) / C_2] \; ; \; s_{44} = 1 / c_{44}$$

$$C_1 = [c_{33}(c_{11} + c_{12}) - 2\, c_{13}{}^2] \; ; \; C_2 = [c_{66}(c_{11} - c_{12}) - 2\, c_{16}{}^2]$$

These are inverted simply by an interchange of symbols $c_{\lambda\mu}$ and $s_{\lambda\mu}$. When c_{16} is set equal to zero in the above equations, the six relations for classes 4-bar, 4, and 4/m are recovered as:

$$s_{11} = [c_{11}c_{33} - c_{13}{}^2] / [(c_{11} - c_{12})\, C_1]$$

$$s_{12} = - [c_{12}c_{33} - c_{13}{}^2] / [(c_{11} - c_{12})\, C_1]$$

$$s_{13} = - [c_{13} / C_1]; \; s_{33} = [(c_{11} + c_{12}) / C_1]$$

$$s_{44} = 1 / c_{44} \; ; \; s_{66} = 1 / c_{66}$$

Definition of Poisson's Ratio for Crystals

Poisson's ratio for crystals is defined in general as $\nu_{ji} = s_{ij}' / s_{jj}'$, where x_j is the direction of the longitudinal extension, x_i is the direction of the accompanying lateral contraction, and the s_{ij}' and s_{jj}' are the appropriate elastic compliances referred to this right-handed axial set. It suffices to take x_1 as the direction of the longitudinal extension; then two Poisson's ratios are defined by the orientations of the lateral axes x_2 and x_3: $\nu_{21} = s_{12}' / s_{11}'$ and $\nu_{31} = s_{13}' / s_{11}'$. Application of the definition requires specification of the orientation of the x_k coordinate set with respect to the crystallographic directions, and transformation of the compliances accordingly.

Relations for Rotated Tetragonal Compliances - General

The unprimed compliances are referred to a set of right-handed orthogonal axes related to the crystallographic axes in the manner defined by the IEEE standard. Direction cosines a_{mn} relate the transformation from these axes to the set specifying the directions of the longitudinal extension (x_1), and the lateral contractions (x_2 and x_3). General expressions for the transformed compliances that enter the formulas for ν_{21} and ν_{31}, including the s_{16} terms, are:

$$\begin{aligned} s_{11}' = {} & s_{11}[a_{11}^4 + a_{12}^4] + s_{33}[a_{13}^4] + (s_{44} + 2s_{13})[a_{13}^2][a_{11}^2 + a_{12}^2] + \\ & (s_{66} + 2s_{12})[a_{11}^2 a_{12}^2] + 2s_{16}[a_{11}a_{12}][a_{11}^2 - a_{12}^2] \end{aligned}$$

$$\begin{aligned} s_{12}' = {} & s_{11}[a_{11}^2 a_{21}^2 + a_{12}^2 a_{22}^2] + s_{33}[a_{13}^2 a_{23}^2] + s_{44}[a_{13}a_{23}][a_{12}a_{22} + a_{11}a_{21}] + \\ & s_{66}[a_{11}a_{12}a_{21}a_{22}] + s_{12}[a_{11}^2 a_{22}^2 + a_{12}^2 a_{21}^2] + \\ & s_{13}[a_{23}^2(a_{11}^2 + a_{12}^2) + a_{13}^2(a_{21}^2 + a_{22}^2)] + \\ & s_{16}[a_{21}a_{22}(a_{11}^2 - a_{12}^2) + a_{11}a_{12}(a_{21}^2 - a_{22}^2)] \end{aligned}$$

$$\begin{aligned} s_{13}' = {} & s_{11}[a_{11}^2 a_{31}^2 + a_{12}^2 a_{32}^2] + s_{33}[a_{13}^2 a_{33}^2] + s_{44}[a_{13}a_{33}][a_{12}a_{32} + a_{11}a_{31}] + \\ & s_{66}[a_{11}a_{12}a_{31}a_{32}] + s_{12}[a_{11}^2 a_{32}^2 + a_{12}^2 a_{31}^2] + \\ & s_{13}[a_{33}^2(a_{11}^2 + a_{12}^2) + a_{13}^2(a_{31}^2 + a_{32}^2)] + \\ & s_{16}[a_{31}a_{32}(a_{11}^2 - a_{12}^2) + a_{11}a_{12}(a_{31}^2 - a_{32}^2)] \end{aligned}$$

Single-Axis Rotations

The general rotation relations given above for s_{11}', s_{12}', and s_{13}' simplify considerably for single-axis rotations. Longitudinal extension is along the x_1 axis; abbreviations $c(\varphi)$ and $s(\varphi)$ stand for $\cos(\varphi)$ and $\sin(\varphi)$, etc.:

(A) Rotation about x_1: $s_{11}' = s_{11}$

$$s_{12}' = s_{12}\,[c^2(\theta)] + s_{13}\,[s^2(\theta)] = s_{12} + (s_{13} - s_{12})[s^2(\theta)]$$

$$s_{13}' = s_{13}\,[c^2(\theta)] + s_{12}\,[s^2(\theta)] = s_{13} + (s_{12} - s_{13})[s^2(\theta)]$$

$$\nu_{21} = \{s_{12} + (s_{13} - s_{12})[s^2(\theta)]\} / s_{11} \;;\; \nu_{31} = \{s_{13} + (s_{12} - s_{13})[s^2(\theta)]\} / s_{11}$$

These expressions are independent of s_{16}, and have two-fold symmetry. When $\theta = \pi/4$, $\nu_{21} = \nu_{31} = (s_{12} + s_{13}) / 2\,s_{11}$

(B) Rotation about x_2:

$$s_{11}' = s_{11}\,[c^4(\psi)] + s_{33}\,[s^4(\psi)] + (s_{44} + 2\,s_{13})[c^2(\psi)s^2(\psi)]$$

$$s_{12}' = s_{12}\,[c^2(\psi)] + s_{13}\,[s^2(\psi)] = s_{12} + (s_{13} - s_{12})[s^2(\psi)]$$

$$s_{13}' = s_{13} + s_2\,[c^2(\psi)\,s^2(\psi)]\,;\; s_2 = (s_{11} + s_{33} - (s_{44} + 2\,s_{13}))$$

$$\nu_{21} = s_{12}' / s_{11}'\,;\; \nu_{31} = s_{13}' / s_{11}'$$

These expressions are independent of s_{16}, and have two-fold symmetry. When $\psi = \pi/4$, $\nu_{21} = 2\,(s_{12} + s_{13}) / (s_0 + s_{44})$

$$\nu_{31} = (s_0 - s_{44}) / (s_0 + s_{44})\,;\; s_0 = (s_{11} + s_{33} + 2\,s_{13})$$

When $\psi = \pi/2$, $\nu_{21} = \nu_{31} = s_{13} / s_{33}$; Poisson's ratio is isotropic when the longitudinal extension is along the four-fold symmetry axis.

(C) Rotation about x_3: $s_{11}' = [s_{11} + F(\varphi)]$; $s_{12}' = [s_{12} - F(\varphi)]$

$$F(\varphi) = [c(\varphi)s(\varphi)]\{s_1[c(\varphi)s(\varphi)] + 2\,s_{16}[c^2(\varphi) - s^2(\varphi)]\}$$

$$s_1 = (s_{66} + 2\,s_{12} - 2\,s_{11})\,;\; s_{13}' = s_{13}$$

$$\nu_{21} = [s_{12} - F(\varphi)] / [s_{11} + F(\varphi)]\,;\; \nu_{31} = s_{13} / [s_{11} + F(\varphi)]$$

When $\varphi = \pi/4$, s_{16} does not appear:

$$\nu_{21} = [4\,s_{12} - s_1] / [4\,s_{11} + s_1]\,;\; \nu_{31} = 4\,s_{13} / [4\,s_{11} + s_1]$$

Transformation Matrix for General Rotations

In order to derive the Poisson's ratio for the most general case, we consider the transformation matrix for a combination of three coordinate rotations: a first rotation about x_3 by angle φ, a second rotation about the new x_1 by angle θ, and a third rotation about the resulting x_2 by angle ψ. When these angles are set to zero, the x_1, x_2, x_3 axes coincide respectively with the reference crystallographic directions. For nonzero angles, the direction cosines a_{mn} are as follows:

$$
\begin{array}{lll}
[c(\varphi)c(\psi) - s(\varphi)s(\theta)s(\psi)] & [s(\varphi)c(\psi) + c(\varphi)s(\theta)s(\psi)] & [-c(\theta)s(\psi)] \\
[-s(\varphi)c(\theta)] & [c(\varphi)c(\theta)] & [\ s(\theta)\ ] \\
[c(\varphi)s(\psi) + s(\varphi)s(\theta)c(\psi)] & [s(\varphi)s(\psi) - c(\varphi)s(\theta)c(\psi)] & [\ c(\theta)c(\psi)]
\end{array}
$$

Substitution of these a_{mn} into the expressions for s_{11}', s_{12}', and s_{13}', and thence into the formulas $\nu_{21} = s_{12}' / s_{11}'$ and $\nu_{31} = s_{13}' / s_{11}'$ formally solves the problem for specified values of φ, θ, and ψ.

Poisson's Ratios for Specific Orientations

1) Longitudinal extension along an axis normal to the four-fold symmetry axis: $\psi = 0$; φ and θ arbitrary. Direction cosines are:

$$
\begin{array}{lll}
[c(\varphi)] & [s(\varphi)] & [\ 0\ ] \\
[-s(\varphi)c(\theta)] & [c(\varphi)c(\theta)] & [s(\theta)] \\
[s(\varphi)s(\theta)] & [-c(\varphi)s(\theta)] & [c(\theta)]
\end{array}
$$

Rotated compliances are:

$$s_{11}' = s_{11} + F(\varphi)$$

$$s_{12}' = s_{12} + (s_{13} - s_{12})[s^2(\theta)] - F(\varphi)[c^2(\theta)]$$

$$s_{13}' = s_{13} + (s_{12} - s_{13})[s^2(\theta)] - F(\varphi)[s^2(\theta)]$$

$$\nu_{21} = [s_{12} + (s_{13} - s_{12})[s^2(\theta)] - F(\varphi)[c^2(\theta)]] / [s_{11} + F(\varphi)]$$

$$\nu_{31} = [s_{13} + (s_{12} - s_{13})[s^2(\theta)] - F(\varphi)[s^2(\theta)]] / [s_{11} + F(\varphi)]$$

When $\varphi = 0$ or $\pi/2$, $F(\varphi) = 0$; case (A). When $\varphi = \pi/4$, $F(\varphi) = s_1 / 4$, and

$$\nu_{21} = [4\, s_{12} + 4\,(s_{13} - s_{12})[s^2(\theta)] - s_1\,[c^2(\theta)]] \,/\, [4\, s_{11} + s_1]$$

$$\nu_{31} = [4\, s_{13} + 4\,(s_{12} - s_{13})[s^2(\theta)] - s_1\,[s^2(\theta)]] \,/\, [4\, s_{11} + s_1]$$

2) Longitudinal extension along an axis not normal to the four-fold symmetry axis, but with x_2 normal to the four-fold symmetry axis: $\theta = 0$; φ and ψ arbitrary. Direction cosines are:

$[c(\varphi)c(\psi)]$	$[s(\varphi)c(\psi)]$	$[-\, s(\psi)]$
$[-\, s(\varphi)]$	$[c(\varphi)]$	$[\;0\;]$
$[c(\varphi)s(\psi)]$	$[s(\varphi)s(\psi)]$	$[\;c(\psi)]$

Rotated compliances are:

$$s_{11}' = [s_{11} + F(\varphi)][c^4(\psi)] + [s^2(\psi)]\{s_{33}[s^2(\psi)] + (s_{44} + 2\, s_{13})[c^2(\psi)]\}$$

$$s_{12}' = s_{12}[c^2(\psi)] + s_{13}[s^2(\psi)] - F(\varphi)[c^2(\psi)]$$

$$s_{13}' = s_{13} + (s_2 + F(\varphi))[c^2(\psi)s^2(\psi)]$$

$$\nu_{21} = s_{12}' / s_{11}' \,;\; \nu_{31} = s_{13}' / s_{11}'$$

When $\psi = \pi/4$, $s_{11}' = [s_0 + s_{44} + F(\varphi)] / 4$:

$$s_{12}' = [s_{12} + s_{13} - F(\varphi)] / 2 \,;\; s_{13}' = [4\, s_{13} + s_2 + F(\varphi) / 4$$

$$\nu_{21} = 2\, [s_{12} + s_{13} - F(\varphi)] \,/\, [s_0 + s_{44} + F(\varphi)]$$

$$\nu_{31} = [4\, s_{13} + s_2 + F(\varphi)] \,/\, [s_0 + s_{44} + F(\varphi)]$$

When $\psi = \pi/2$, $s_{11}' = s_{33}$; $s_{12}' = s_{13}$; $s_{13}' = s_{13}$:

$$\nu_{21} = \nu_{31} = s_{13} / s_{33}$$

Conclusions

Poisson's ratio, with respect to rotated coordinate axes for tetragonal materials, has been obtained. Four cases are of particular interest:

- For longitudinal extension along x_1, and x_3 along the four-fold symmetry axis: $\nu_{21} = s_{12} / s_{11}$; $\nu_{31} = s_{13} / s_{11}$

- For longitudinal extension along an axis bisecting the original x_1 and x_3 axes; x_2 normal to the four-fold symmetry axis:

$$\nu_{21} = 2(s_{12} + s_{13}) / (s_0 + s_{44})$$

$$\nu_{31} = (s_0 - s_{44}) / (s_0 + s_{44})$$

- For longitudinal extension along the four-fold symmetry axis, the result is independent of the azimuthal angle φ:

$$\nu_{21} = \nu_{31} = s_{13} / s_{33}$$

- For longitudinal extension along an axis bisecting the original x_1 and x_2 axes, and x_3 along the four-fold symmetry axis:

$$\nu_{21} = [4\, s_{12} - s_1] / [4\, s_{11} + s_1]$$

$$\nu_{31} = 4\, s_{13} / [4\, s_{11} + s_1]$$

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